Methallyl alcohol 513-42-8 | DTXSID4060155

Model	Performance
IVIOGCI	1 CHOHILANCE

Model	Data	

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 6.73 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.44e-01

Confidence level: 7.74e-01

Nearest Neighbors from the Training Set

Image not found

2-Methylpent-1-ene Measured: 3.55 Predicted: 61.0 Image not found

Ethylenediamine Measured: 26.1 Predicted: 6.61 Image not found

Diacetone alcohol Measured: 2.37 Predicted: 1.27

Image not found

Isobutylamine Measured: 10.4 Predicted: 172 Image not found

Barbituric acid Measured: 6.70 Predicted: 4.85e-08